Biographical Sketch Krishnan Balasubramanian

http://www.public.asu.edu/~baluk/main.htm

A. Professional Preparation: Birla Institute of Technology & Science, Pilani India 1977 MSc (Hons) with Distinction
The Johns Hopkins University 1980 M.A. & PhD
Post-doc, Lawrence Berkeley Lab, University of California, Berkeley 1980-1983

B. Appointments: http://www.public.asu.edu/~baluk/credent.html
Lawrence Livermore National Laboratory, and , Lawrence Berkeley National Laboratory, UC Berkeley, Senior Scientist 2000-
Adjunct Professor, Dept. of Mathematics & Computer Science, California State University East Bay, CA 2005-
University of California (UC), Davis, Department of Applied Science,

Step VI Professor 2000-2005
Arizona State University
Professor Emeritus 2000- Professor
1990-2000
Associate Professor 1987-1989
Assistant Professor 1983-1986
Distinguished Professor, Birla Institute of Technology & Science, Pilani, Rajasthan, India
Distinguished Professor, SRM University, India
Adjunct Professor University of Houston, Houston TX till 2014
Distinguished Professor, Indian Institute of Science, Bangalore, India Spring 1997

Honors and Awards http://www.public.asu.edu/~baluk/award.html

Elected Member of International Academy of Mathematical Chemistry 2004

Elected Member EU Academy of Sciences

National Academy of Sciences, Advisory Panelist
Chemistry and Materials Science Directorate Associate Director Award, Exceptional Service Award,
Robert S. Mulliken Lecture
IIT Madras, Director Extramural Distinguished Lecture 2005
Joint Prize of Minister of Education, Polish Government 1998
Top 0.1% of most cited Chemists 1986-1997
Fulbright Distinguished Professor Research Award 1996-1997
Award for Distinction in Graduate Teaching 1991
The Camille and Henry Dreyfus Teacher-Scholar Award 1985-1990
Birla Institute of Technology & Science Distinguished Lecturer 1989
Alfred P. Sloan Fellow 1984-1988

Rev Fr. Yeddanapalli Memorial Award 2019
Fulbright Research professor 2016
Padmasri Gemini Ganesan Centennial Lecture
International Poetry Society Award
Phi Kappa Phi & Alpha Chi Sigma
Citation from Institute of Scientific Information as the author of one of most cited 1986 Chemistry papers
National Science Talent Scholar 1973

Journal Editorship

Mathematical & Computational Chemistry (Past)

Current Topics in Medicinal Chemistry, Associate Editor,

Regional Editor (North America) Letters in Drug Design & Discovery

Editorial Advisory Board

Journal of Mathematical Chemistry

Symmetry
Current Computer Aided Drug Discovery
Journal of Mathematical Sciences & Modeling
Biomedicines
Journal of Zhejiang University Science
Journal of Computing Letters
Biochemistry & Modern Applications
EC Pharmacology & Toxicology

Scientific Panels/Advisory Panels

National Academy o Sciences/National Research Council Panelist
Advisory Panel to the Chemical Sciences Division of the Air Force Office of Scientific Research,
DOE panel for the Laboratory Technology Program,
DOE Environmental Management Science Program (EMSP) Panel,
NSF panelist,
DOE-BES Panelist ,
NATO,
Petroleum Research Fund administered by American Chemical Society,
Austrian Science Foundation
The Czech Science Foundation
National Institute of Health
US Environmental Protection Agency

Research Interests http://www.public.asu.edu/~baluk/resch.html

Computational nanotechnology, Development of Engineered mesoporous materials for sensors, Computational Biotechnology, Machine Learning & Artificial Intelligence with applications to Drug Discovery, Graphs, Discrete Math & Applied Computer Science, Computational Actinide Chemistry with applications to energy and environment, Catalysis, Energy Conversion and Hydrogen Storage, Superheavy molecules, Transactinides, Computational Biochemistry & Bioinformatics, Relativistic electronic structure & Quantum Chemistry, and Chemical Applications of Graph theory & Group theory, Fullerenes & Giant Fullerenes, Metal Clusters, Semiconductor Clusters, Water Clusters, Nonrigid Molecules, Computational Spectroscopy.

Recent Research Grants

1. **Engineered Mesoporous Materials for the development of Actinide Detection, Sequestration &Sensors, Department of Homeland Security, $170,000 for FY2012 $1560,000 from 2008-2011 and a Continuing multi-year Grant.**

2. **Electronic Structure of Transition Metal Clusters & Reactivity, and Electronic Structure of Environmental Actinide Complexes, $241,000 for FY2011-2012 , $122,000/ FY2013 and a Continuing multi-year Grant since 1986 with an unprecedented repeat record of renewals continuously from 1986, US Department of Energy, Office of Basic Energy Sciences, Washington, DC**

Publications

G-Scholar Profile

738. Balasubramanian, K. Vertex and Face Colorings of Dodecahedron and its distortions for all Irreducible Representations: Insights into Dynamic Chirality, Pentagonal, Jahn-Teller and elongated Distortions. Journal of Mathematical Chemistry, 2025, in press

737. Balasubramanian, K Combinatorics of Random Walks on Graphs and Walk-Entropies-Generalized Petersen and Isomerization Graphs. Journal of Mathematical Chemistry. 2025

736. Balasubramanian, K Spectral Polynomials and Spectra of graphs beyond cubic and

Icosahedral symmetries: n-octahedra, n-cubes, symmetric and semi-symmetric graphs, Giant Fullerene cages and Generalized Petersen Graphs. Symmetry, 2025

735. Balasubramanian, K Matching Polynomials of Symmetric, Semisymmetric, Double Group Graphs, Polyacenes, Wheels, Fans, and symmetric solids in third and higher dimensions. Symmetry, 2025

734. Micheal Arockiaraj, J. Celin Fiona, S. Prabhu, S. Vijay, R. San Diego, Krishnan Balasubramanian,Topological, Graph-Spectral, Entropy Properties, NMRand ESR Spectral Patterns of Hydrogen-BondedNanosheets of Boric Acid, J. Cluster Sci. 2025,

733. Rakhi Yadav; Dhivya Antony; B.P.Anisha Aravind; Krishnan Balasubramanian; Mullai kodi R K , A Computational and Experimental reflection on Green-Synthesized CaO and Selenium-Doped CaO Nanoparticles: Spectral Analysis, Structural Insights, and Apoptotic Impacts, Chemistry Select 2025,

732. Kavin Jacob, Joseph Clement ,Micheal Arockiaraj, Pancras Peter, Krishnan Balasubramanian Network topology and entropy analysis of tetragonal farneseite zeolites, Nature, Scientific Reports 2025,

731. Balasubramanian, K. Enumeration of n-Dimensional Hypercubes, Icosahedra, Rubik's Cube Dice, Colorings, Chirality, and Encryptions Based on Their Symmetries. Symmetry 2024, 16, 1020. https://doi.org/10.3390/sym16081020

730. Arockiaraj, M.; Raza, Z.; Maaran, A.; Abraham, J.; Balasubramanian, K. Comparative analysis of scaled entropies and topological properties of triphenylene-based metal and covalent organic frameworks. Chemical Papers, 2024, 78(7), 4095–4118.

729. Balasubramanian, K. New Insights into Aromaticity through Novel Delta Polynomials and Delta Aromatic Indices. Symmetry 2024, 16, 391. https://doi.org/10.3390/sym16040391

728. Medha Itagi Huilgol, P.H. Shobha, Krishnan Balasubramanian, Novel topological reverse indices and entropies of armchair versus zigzag polyhex carbon nanotubes with spectroscopic applications,Computational and Theoretical Chemistry, 2024, 1242,114921, https://doi.org/10.1016/j.comptc.2024.114921.

727. Micheal Arockiaraj, J. Celin Fiona, Krishnan Balasubramanian, Degree based hybrid topological indices and entropies of hydrogen bonded benzo-trisimidazole frameworks, Journal of Molecular Structure,2024, 1314, 138740, https://doi.org/10.1016/j.molstruc.2024.138740.

726. Arockiaraj, M., Jency, J., Shalini, A.J. Balasubramanian, K. Degree-based topological insights and graph entropies of Kagome lattice covalent organic frameworks. Chem. Pap. (2024). https://doi.org/10.1007/s11696-024-03743-5

725. Arockiaraj, M., Fiona, J.C., Arokiya Doss, C.I. Balasubramanian, K. Mathematical techniques for graph descriptors, entropies, spectra, and properties of oxalate-based metal organic frameworks. Journal of Mathematical Chemistry, 2024, pp.1-29.

724. Prabhu, S., Arulperumjothi, M., Manimozhi, V. Balasubramanian, K. Topological characterizations on hexagonal and rectangular tessellations of antikekulenes and its computed spectral, nuclear magnetic resonance and electron spin resonance characterizations. International

Journal of Quantum Chemistry, 2024, 124(7), p.e27365.

723. Arockiaraj, M., Fiona, J.C., Abraham, J., Klav�ar, S. Balasubramanian, K. Guanidinium and hydrogen carbonate rosette layers: distance and degree topological indices, Szeged-type indices, entropies, and NMR spectral patterns. Heliyon, 2024, 10(3).

722. Arockiaraj, M., Raza, Z., Fiona, J.C., Abraham, J., Shalini, A.J. Balasubramanian, K. Topological descriptors, entropy measures and NMR spectral predictions for nanoporous graphenes with [14] annulene pores. International Journal of Quantum Chemistry, 2024, 124(1), p.e27284.

721. Arockiaraj, M., Paul, D., Rahul, M.P., Clement, J., Tigga, S. Balasubramanian, K. Topological and Entropy Indices in Qspr Studies of N-Carbophene Covalent Organic Frameworks. BioNanoScience, 2024, 14(3), pp.2762-2773.

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719. Arockiaraj, M.; Jency, J.; Maaran, A.; Abraham, J.; Balasubramanian, K. Refined Degree Bond Partitions, Topological Indices, Graph Entropies and Machine-generated Boron NMR Spectral Patterns of Borophene Nanoribbons., J. Mol. Struc. September 1, 2023, 136524, https://www.sciencedirect.com/science/article/abs/pii/S0022286023016149

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and entropy indices of n-dimensional hypercubes. Journal of Mathematical Chemistry, 2023, 61, 1570-1591.

711. Balasubramanian, K. ; Davidson, E. R. Rational approximations to pie: transcendental pi and Euler's Constant e Journal of Mathematical Chemistry, 2023, 61, 1471-1476.

710. Raza, Z.; Arockiaraj, M.; Maaran, A.; Kavitha,S. R. J.; Balasubramanian, K. Topological entropy characterization, NMR and ESR spectral patterns of coronene-based transition metal organic frameworks. ACS omega 2023, 8 (14), 13371-13383.

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Journal of Molecular Structure **2023**,1277,134786 [PDF]

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Journal of Physical Organic Chemistry, **2022**, e4435 [PDF]

698. Mushtaq, M.; Arockiaraj, M.; Fiona, J. C.; Jency, J.;Balasubramanian, K Topological properties, entropies, stabilities and spectra of armchair versus zigzag coronene-like nanoribbons, *Molecular Physics* **2022**, 120 (17), e2108518 [PDF]

697. Arockiaraj, M.; Jency, J.; Abraham, J.; Ruth Julie Kavitha, S.; Balasubramanian, K Two-dimensional coronene fractal structures: topological entropy measures, energetics, NMR and ESR spectroscopic patterns and existence of isentropic structures. *Molecular Physics,* p.e2079568. **2022**, [PDF]

696. Rahul, M.P.; Clement, J.; Junias, J. S.; Arockiaraj, M.; Balasubramanian, K. Degree-based entropies of graphene, graphyne and graphdiyne using Shannon's approach, *Journal of Molecular Structure* **2022**,1260,132797[PDF]

695. Balasubramanian, K.; Carbo Dorca, R. Three Conjectures on Extended Twin Primes and the Existence of Isoboolean and Singular Primes Inspired by Relativistic Quantum Computing,**?** *Journal of Mathematical Chemistry* **2022**, 60, 1571**?**1583. DOI: 10.13140/RG.2.2.22432.25600, [PDF]

694.Arockiaraj,M.; Mushtaq,S.; Klavzar,S.; Fiona,J.C.; Balasubramanian, K. Szeged-like Topological Indices and the Efficacy of the Cut Method: The Case of Melem Structures, *Discrete Math. Lett.* **2022**,9,49-56 DOI: 10.47443/dml.2021.s209 [PDF]

693. Amrutha, P.; Bakkyaraj, T.; Balasubramanian, K.; T. Geetha, T. Decomposition of Induced Representations of Dihedral Groups (Dn) to Symmetric Groups (Sn): Applications to cyclic nanotubes, Gelfand States, Tableaus and Spectroscopy, J. Math. Chem. **2022,** 60 (4), 733-751. **DOI 10.1007/s10910-022-01325-y** [PDF]

692. Antony, D.; Balasubramanian, K.; Yadav, R. Experimental and Computational Studies of Structures, Spectra and Bioactivities of Phytomediated Selenium-Supported CaO, CuO and ZnO Nanoparticles- Potential Drugs for Breast Cancer, J. Mol. Structure. **2022,** 1263, 133113 [PDF]

691. Arockiaraj, M.; Kavitha, S. R. J..; Klavzar,S.; Fiaona, J. C.; Balasubramanian, Topological Characterization of Cycloparaphenylene Series, *Polycyclic Aromatic Compounds*. **March 13, 2023, 1-23 . https://doi.org/10.1080/10406638.2023.2186442** [PDF]

690. Mushtaq, S.; Arockiaraj, M.; Klavzar,S.; Fiaona, J. C..; Balasubramanian, K.Comment on Mostar indices of SiO2 nanostructures and melem chain nanostructures, *Int. J. Qunat. Chem.* **2022**, 122 (11), e26894 [PDF]

689. Arockiaraj, M.; Paul, D.; Klavzar,S.; Clement, J.; Tigga,S.; Balasubramanian, K. Relativistic distance based and bond additive topological descriptors of zeolite RHO materials, *Journal of Molecular Structure*, **2022**, 1250, Part 2,131798:1-14. [PDF]

688. Abraham, J.; Arockiaraj, M.; Jency, J.; Kavitha, S. R.J.; Balasubramanian, Graph Entropies, Enumeration of Circuits, Walks and Topological Propertiesof Three Classes of Isoreticular Metal Organic Frameworks, *J. Math. Chem.* **2022,** 60 (4), 695-732. **DOI 10.1007/s10910-021-01321-8** [PDF]

687. Balasubramanian, K. Symmetry and Combinatorial Concepts for Cyclopolyarenes, Nanotubes and 2D-sheets: Enumerations: Isomers, Structures & Properties Symmetry **2022,** 14 (1), 34[PDF]

686. Medha Itagi Huilgol, V. Sriram & Krishnan Balasubramanian (**2021**) Structure-activity relations for antiepileptic drugs through omega polynomials and topological indices, *Molecular Physics*, **2022**,120 (3), e1987542:1-24 [PDF]

685. Balasubramanian, K. Symmetry, Combinatorics, Artificial Intelligence, Music and Spectroscopy. *Symmetry* **2021**, 13, 1850:1-44. [PDF]

684. Kavitha, S.R.J.; Abraham, J., Arockiaraj, M.; Jency, J.; Balasubramanian, K., **2021**. Topological Characterization and Graph Entropies of Tessellations of Kekulene Structures: Existence of Isentropic Structures and Applications to Thermochemistry, Nuclear Magnetic Resonance, and Electron Spin Resonance. *The Journal of Physical Chemistry A*, **2021**, 125(36), 8140-8158. [PDF]

683. Balasubramanian, K.; Ottorino, O.; Cataldo, F.; Putz, M. V. Combinatorics of chiral and stereo isomers of substituted nanotubes: applications of Eulerian character indices and comparison with bondonic formalism, *Fullerenes, Nanotubes and Carbon Nanostructures*, **2022,** 30 (3) 315-333[PDF]

682. Balasubramanian, K. Combinatorial enumeration of stereo, chiral and position isomers of polysubstituted halocarbons: applications to machine learning of proton and 35Cl NMR spectroscopy of halocarbons. *Theor Chem Acc* **2021**, 140, 58:1-26. [PDF]

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679. Huilgol, M.I., Divya, B. & Balasubramanian, K. Distance degree vector and scalar sequences of corona and lexicographic products of graphs with applications to dynamic NMR and dynamics of nonrigid molecules and proteins. Theor Chem Acc **2021**,140, 25:1-26. https://doi.org/10.1007/s00214-021-02719-y [PDF]

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674. Arockiaraj, M., Prabhu, S., Arulperumjothi, M. et al. Correction to: Topological characterization of hexagonal and rectangular tessellations of kekulenes as traps for toxic heavy metal ions. Theor Chem Acc **2021**, 140, 112 [PDF]

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672. Patil M. Vaishali , Narkhede R. Rohan,Masand Neeraj ,Cheke S. Rameshwar , Balasubramanian Krishnan, Molecular Insights into Resveratrol and Its Analogs as SARS-CoV-2 (COVID-19) Protease Inhibitors , Coronaviruses **2021**; 2(11) : e130921189258. [PDF]

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669. Balasubramanian, K.; Ori, O., Cataldo, F., Ashrafi, A. R. Face Colorings and Chiral Face Colorings of Icosahedral Giant Fullerenes: C80 to C240 , *Fullerenes, Nanotubes and Carbon Nanostructures* **2021**, 29:1, 1-12, DOI: 10.1080/1536383X.**2020**.1794853. [PDF]

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665. Arockiaraj M, Klavzar S, Mushtaq S, Balasubramanian K. Topological Characterization of the Full k-Subdivision of a Family of Partial Cubes and Their Applications to α-Types of Novel Graphyne and Graphdiyne Materials. *Polycyclic Aromatic Compounds.* **2021**, 41:9, 1902-1924. [PDF]

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